

Membrane protein FhaC:

During this run on ID14-4, we have measured three data sets on two different types of crystals that reflect two conformational states of the protein.

- 2 data sets have been measured on crystals obtained with the protein which has never secreted the FHA adhesin (crystals named FhaCbe)
- 1 data set has been measured on a crystal obtained with the protein extracted after it had secreted the FHA protein. (crystals named FhaCaf)

We have tried to solve the structure by SAD using crystals FhaCbe, that were obtained in the presence of HG in the crystallization buffer. Unfortunately, incorporation of HG into these crystals was not sufficient to provide us with an exploitable phasing signal. We thank our beamline contact (Dr. Raymond Ravelli) for his help in trying to exploit some phasing signal on these crystals.

Data have been processed with XDS.

Data collection statistics for crystal FhaCbe n° 1:

SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION											
RESOLUTION	NUMBER OF REFLECTIONS			COMPLETENESS	R-FACTOR	R-FACTOR	COMPARED	I/SIGMA	R-meas	Rmrgd-F	S_norm/ S_ano
LIMIT	OBSERVED	UNIQUE	POSSIBLE	OF DATA	observed	expected					
8.58	3671	1323	1390	95.2%	4.0%	3.8%	3624	25.33	5.0%	3.1%	1.12
6.11	6888	2424	2444	99.2%	4.2%	4.3%	6828	20.62	5.2%	4.1%	1.08
5.00	8995	3127	3151	99.2%	4.9%	5.1%	8934	18.19	6.0%	5.2%	1.04
4.34	10581	3671	3705	99.1%	4.6%	5.1%	10507	17.78	5.7%	5.1%	1.02
3.88	12125	4195	4235	99.1%	7.2%	7.3%	12051	12.81	8.9%	9.3%	1.01
3.55	13237	4582	4624	99.1%	13.0%	13.0%	13142	8.25	16.0%	16.8%	1.02
3.29	14460	5001	5065	98.7%	23.2%	23.7%	14357	4.97	28.6%	31.8%	1.03
3.07	15618	5390	5456	98.8%	44.7%	46.7%	15500	2.67	55.1%	64.0%	1.02
2.90	16026	5592	5753	97.2%	65.7%	69.8%	15857	1.81	81.0%	92.6%	1.02
total	101601	35305	35823	98.6%	8.2%	8.5%	100800	9.82	10.2%	17.5%	1.04

Data collection statistics for crystal FhaCbe n° 2:

SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION												
RESOLUTION LIMIT	NUMBER OF REFLECTIONS			COMPLETENESS OF DATA	R-FACTOR observed	R-FACTOR expected	COMPARED	I/SIGMA	R-meas	Rmrgd-F	S_norm/ S_ano	
	OBSERVED	UNIQUE	POSSIBLE									
10.58	1326	702	770	91.2%	1.5%	1.6%	1183	43.09	2.1%	1.6%	1.30	
7.57	2698	1295	1308	99.0%	2.0%	2.0%	2578	33.72	2.7%	2.5%	1.14	
6.21	3540	1688	1698	99.4%	3.1%	3.4%	3379	21.11	4.2%	5.0%	1.08	
5.39	4172	1983	1987	99.8%	4.5%	4.8%	3957	16.17	6.1%	7.2%	1.07	
4.83	4776	2270	2278	99.6%	5.3%	5.3%	4512	14.76	7.1%	8.3%	1.05	
4.41	5192	2457	2465	99.7%	5.6%	5.5%	4889	14.17	7.5%	8.9%	1.03	
4.09	5699	2706	2722	99.4%	9.9%	9.7%	5349	8.77	13.2%	16.3%	1.03	
3.82	6069	2882	2893	99.6%	16.2%	16.5%	5680	5.49	21.7%	27.1%	1.05	
3.61	6422	3061	3099	98.8%	27.9%	27.8%	5986	3.32	37.3%	45.1%	1.04	
total	39894	19044	19220	99.1%	5.2%	5.3%	37513	13.64	7.0%	12.0%	1.07	

Data collection statistics for crystal FhaCaf:

SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION												
RESOLUTION LIMIT	NUMBER OF REFLECTIONS			COMPLETENESS OF DATA	R-FACTOR observed	R-FACTOR expected	COMPARED	I/SIGMA	R-meas	Rmrgd-F	S_norm/ S_ano	
	OBSERVED	UNIQUE	POSSIBLE									
11.65	1233	500	541	92.4%	4.2%	5.4%	1182	15.93	5.4%	4.0%	1.12	
8.37	2265	902	915	98.6%	7.0%	6.4%	2186	12.85	8.8%	7.2%	1.08	
6.87	2939	1160	1168	99.3%	10.7%	10.0%	2844	8.13	13.5%	12.2%	1.02	
5.96	3534	1389	1397	99.4%	17.9%	18.6%	3413	4.85	22.5%	20.9%	1.02	
5.34	4000	1570	1576	99.6%	23.5%	25.0%	3854	3.84	29.6%	27.3%	1.00	
4.88	4337	1698	1706	99.5%	27.4%	28.6%	4194	3.43	34.4%	29.5%	1.01	
4.52	4793	1867	1872	99.7%	27.3%	26.2%	4633	3.64	34.0%	31.8%	1.01	
4.23	4987	1993	1995	99.9%	31.3%	29.6%	4807	3.03	39.1%	36.4%	1.02	
3.99	4934	2011	2147	93.7%	44.0%	49.1%	4676	2.02	55.2%	49.6%	1.02	
total	33022	13090	13317	98.3%	16.5%	16.9%	31789	4.93	20.8%	24.4%	1.03	